Glass Relaxation is Controlled by the Topology of the Atomic Network

Hu, Yushu; Li, X.; Song, W.; Liu, Z.; Bechgaard, Tobias Kjær; Smedskjær, Morten Mattrup; Bauchy, Mathieu

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Y. Hu[1]; X. Li[1]; W. Song[1]; Z. Liu[1]; T. K. Bechgaard[2]; M. M. Smedskjaer[2]; M. Bauchy[*1]

1. University of California, Los Angeles, Civil and Environmental Engineering Department, USA 2. Aalborg University, Denmark

Understanding, predicting, and controlling glass relaxation is of primary importance for the manufacturing of display glasses, as any small variation in volume can result in undesirable pixel misalignments. However, no clear atomistic mechanism of structural and stress relaxation is available to date, which limits our ability to identify optimal glass compositions featuring low relaxation. Here, based on molecular dynamics simulations, we study the relaxation of a series of alkali-free calcium aluminosilicate (CAS) and sodium silicate (NS) glasses with varying compositions. We observe that selected glass compositions exhibit minimal relaxation. We investigate the structural origin of this behavior by means of topological constraint theory. Based on this analysis, we demonstrate that minimal relaxation is achieved for isostatic glasses, which are both free of eigenstress and floppy modes. This highlights the crucial role of the atomic topology in controlling the propensity for relaxation.